A Markov Chain-Based Numerical Method for Calculating Network Degree Distributions [*]

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Abstract

This paper establishes a relation between scale-free networks and Markov chains, and proposes a computation framework for degree distributions of scale-free networks. We first find that, under the BA model, the degree evolution of individual nodes in a scale-free network follows some non-homogeneous Markov chains. Exploring the special structure of these Markov chains, we are able to develop an efficient algorithm to compute the degree distribution numerically. The complexity of our algorithm is $O(t^2)$, where t is the number of time steps for adding new nodes. We use three examples to demonstrate the computation procedure and compare the results with those from the existing methods.

PACS: 84.35.+i; 64.60.Fr; 87.23.GE

Keywords: scale-free network, Markov chain, numerical method, degree distribution, degree exponent, degree coefficient

1 Introduction

Complex networks describe a wide range of practical systems of high technological, biological, and social importance [1,2]. For example, the Internet, the World Wide Web (WWW), biological cells and communities of scientists can all be described as complex networks.

Erdös and Rényi [3] started the early studies of complex networks as random graphs in 1960. Many years later, Watts and Strogats [4]'s construction of the small-world network in 1998 represents an interesting development for the study of complex networks

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in that it was motivated by observations of real system behaviors (e.g., Milgram's six-degree connectivity [5]). A common feature of the random graph and small-world models is that the degree distribution (the probability of finding a node with k connections) decays exponentially with the number of connections. However, empirical evidences from the Internet and WWW, among other complex networks, show a fundamentally different picture, i.e., the tail of the degree distribution follows a power law. This led to the introduction in 1999 of scale-free networks by Albert, Barabaási, and Jeong in their pioneering works [6-8], and the start of a new phase in the study of complex networks. Recent studies [9-20] are characterized by empirical observations of scale-free behaviors in various practical systems and investigations of the formation mechanisms of scale-free network. A number of important properties in scale-free networks have been identified, such as the small-world character, the emergence of hubs, and robustness and frangibility. These properties show that scale-free networks can play an important role in the understanding of many complex and important systems.

Two general features can be observed in many real-world networks: successive additions of new nodes and certain preference in linking to existing nodes. Albert, Barabaási, and Jeong proposed two mechanisms to characterize the evolution of a scale-free network [7, 8]: the growth mechanism, starting from m_0 nodes, the network grows at a constant speed, i.e., adding one node at each time step and connecting to $m(m \leq m_0)$ existing nodes; the preferential attachment, the chance that an existing node receives a connection from a new node is proportional to the number of connections it already has. The authors show that, under these two mechanisms, a network evolves into a stationary scale-free state. Its degree distribution follows a power law with the degree exponent $\gamma = 2.9 \pm 0.1$ from simulation analysis and $\gamma = 3$ from the analytical result. These results are significant for complex networks and the two mechanisms become the first model, referred to as the BA model, by which large networks can self-organize into a stationary scale-free state. Empirical evidences show that in many networks, the number of edges grows faster than the number of nodes. This leads to the investigations of m-varying BA models, such as Dorogovtsev and Mendes [20].

Our research is mainly motivated by the following observation. While analytical solutions of the degree distribution for some simple models, such as the BA model, can usually be obtained, one has to resort to simulation for the degree distribution when the mechanisms in model become more complex. This may inhibit the further development of the theory on complex networks. In this paper, we propose an alternative approach. We first find that the degree evolution of a complex network can be characterized by a sequence of Markov chains. By carefully analyzing the structure of these Markov chains, we then develop an efficient numerical method to compute the degree distribution of complex network models. To show the feasibility and efficiency of our numerical method, we compute the degree distribution of the basic BA model and two of its variants.

We organize the paper as follows. In the next section, we review some of the existing methods for network degree distributions. We then use Markov chains to capture network dynamics. Exploring the special structure of the transition matrices of the Markov chains, we develop an efficient algorithm to compute the degree distribution asymptotically. We use this algorithm to compute the exponent of the degree distribution of the BA model. In Section 3, we compute the degree distributions of two m-varying BA models. We verify our approach by showing that our numerical results for the BA model and its variants match very closely to the existing results from the analytical and simulation approaches. We conclude the paper in Section 4 by pointing out some future research opportunities.

2   A Markov chain-based numerical method

With the preferential attachment mechanism of the BA model, the probability that node i receives a connection from an up coming new node is proportional to its own

degree k_i [7], i.e.,

$$\Pi(k_i) = \frac{k_i}{\sum_j k_j}. \tag{1}$$

Assuming continuity of $k_i(t)$ and treating $\Pi(k_i)$ as its rate of growth, $k_i(t)$ then satisfies the following dynamic equation [7, 8]

$$\frac{\partial k_i}{\partial t} = m\Pi(k_i) = m\frac{k_i}{\sum_j k_j} = \frac{k_i}{2t}. \tag{2}$$

Under the initial condition that $k_i(t_i) = m$, the solution of this equation leads to

$$k_i(t) = m(\frac{t}{t_i})^\beta \quad , \quad \beta = \frac{1}{2} \tag{3}$$

where t_i is the time when node i joins the network, and the degree distribution

$$P(k) \sim 2m^2 k^{-\gamma} \quad , \quad \gamma = 3. \tag{4}$$

Here, β is called the dynamic exponent while γ the degree exponent.

The above simple analytical method is often refereed to as the continuum (mean field) theory. Similar power law results for the degree distribution are also obtained using different analytical methods by other authors. For example, with the master-equation approach [14], Dorogovtsev, Mendes and Samukhin treat the degree $k_i(t)$ of a node i at a fixed time t as a random variable. Thus its probability $P(k, t_i, t)$ for the BA model has the following relation:

$$P(k, t_i, t+1) = \frac{k-1}{2t}P(k-1, t_i, t) + (1 - \frac{k}{2t})P(k, t_i, t). \tag{5}$$

Let

$$P(k, t) = \frac{\sum_{t_i} P(k, t_i, t)}{t}. \tag{6}$$

Assuming that the limit $P(k) = \lim_{t \to \infty} P(k, t)$ exists and $\lim_{t \to \infty} t[P(k, t+1) - P(k, t)] = 0$ (this is an additional condition), the degree distribution satisfies equation:

$$2P(k) - 2\delta_{k,m} = (k-1)P(k-1) - kP(k), \tag{7}$$

and the network degree distribution can be obtained as

$$P(k) = \frac{2m(m+1)}{k(k+1)(k+2)}. \tag{8}$$

Krapivsky, Redner and Leyvraz's rate-equation approach [15] focuses on the number $N_k(t)$ of nodes with k edges at time t. For the BA model, $N_k(t)$ is shown to satisfy

$$\frac{dN_k}{dt} = m\frac{(k-1)N_{k-1}(t) - kN_k(t)}{\sum_k kN_k(t)} + \delta_{k,m}. \tag{9}$$

Asymptotically, $N_k(t) = tP(k)$ and $\sum_k kN_k(t) = 2mt$, leading to equation (7).

While the above methods handle simple models, such as the BA model, well, they do not, so far from the best of our knowledge, render analytical solutions for more complicated models. In this case, one can usually use simulation. While simulation is widely applicable, it is usually quite time consuming and may not be flexible enough for in-depth analysis of network behaviors. Here, we propose a different approach to capture the network dynamics.

Consider the degree $K_i(t)$ of node i at time t. Following the increase of t, the sequence $\{K_i(t), t = i, i+1, ...\}$ is, based on the preferential attachment mechanism of the BA model, a stochastic process with the state space $\Omega = \{m, m+1, ...\}$. Here and

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below, we use the upper case K to emphasize the fact that the degree sequence is a stochastic process. The attachment mechanism also indicates that the future evolution of the process is independent of the past history, given its current state; but it is time-dependent. This shows that the process $\{K_i(t)\}$ is in fact a non-homogeneous Markov chain [21], with time-dependent transition probability

$$p_{kj}(t+1) = P\{K_i(t+1) = j \mid K_i(t) = k\} = \begin{cases} 1 - \frac{k}{2t}, & j = k \\ \frac{k}{2t}, & j = k+1 \\ 0, & otherwise \end{cases} \qquad (10)$$

for $k = m, ..., m+t-i$, and

$$p_{kj}(t+1) = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \qquad (11)$$

for $k > m+t-i$. Thus, the dynamics of a node from the time it joins the network is described by a non-homogeneous Markov chain and the whole network (excluding the original nodes) is completely described by t non-homogeneous Markov chains, where t is the time of the observation. Let $P_i(t+1)$ be the one-step transition probability matrix of node i at time t. We have, for $t = i, i+1, ...$

$$P_i(t+1) = \begin{bmatrix} 1 - \frac{m}{2t} & \frac{m}{2t} & & & & \\ & 1 - \frac{m+1}{2t} & \frac{m+1}{2t} & & & \\ & & \ddots & \ddots & & \\ & & & 1 - \frac{m+t-i}{2t} & \frac{m+t-i}{2t} & \\ & & & & 1 & 0 \\ & & & & & \ddots & \ddots \end{bmatrix}. \qquad (12)$$

Let $f_i(t)$ be the probability vector (distribution) of $K_i(t)$ for a given t, and

$$F_{t+1}^{(S,T)} = \sum_{i=S}^{T} f_i(t+1), \quad P(k,t+1) = \frac{F_{t+1}^{(S,t)}(k-m+1)}{t-S+1}. \qquad (13)$$

Here, S and T are two fixed integers between 1 and t. Their meanings will be clear in the computation procedure later. The desired degree distribution of the network is then $P(k) = \lim_{t \to \infty} P(k, t+1)$.

Let us examine (13) to see what is involved in computing the network degree distribution. It is clear that $P\{K_i(i) = k\} = 1$ if $k = m$ and 0 otherwise. We then have the initial probability vector

$$f_i(i) = (1, 0, 0, ...) = e_1 \qquad (14)$$

for any i. By density evolution of Markov chain, the $t+1$-step probability vector $f_i(t+1)$ is given by

$$f_i(t+1) = e_1 \cdot P_i(i+1) \cdot P_i(i+2) \cdots P_i(t+1) , \quad t = i, i+1, ... \qquad (15)$$

where the dots represent matrix multiplications. This, together with (13), shows that computing the degree distribution requires the multiplications and summations of an infinite number of infinite matrices. It is not realistic to expected any meaningful analytical solution from these computations. Even numerical computation seems unmanageable. Fortunately, our past experience in infinite matrix computations [22] with a rectangle-iterative algorithm guides us to explore the special structure of the one-step transition matrices. This leads to dramatically simplified matrix manipulations and a highly efficient algorithm.

We note that while the transition matrices of consecutive nodes are different, their structural similarities lead to the following relations

$$e_1 P_i(t) = e_1 P_1(t), \quad i = 2, 3, ...; \quad t = i + 1, i + 2, ... \tag{16}$$

$$e_1 P_i(t) P_i(t+1) = e_1 P_1(t) P_1(t+1), \quad i = 2, 3, ...; t = i + 1, i + 2, ... \tag{17}$$

and in general

$$e_1 P_i(t) P_i(t+1) \cdots P_i(t+s) = e_1 P_1(t) P_1(t+1) \cdots P_1(t+s), \tag{18}$$

for $i = 2, 3, ...$; $t = i + 1, i + 2, ...$ and $s = 2, 3, ...$. Substituting the above relations into

$$F_{t+1}^{(S,T)} = \sum_{i=S}^{T} f_i(t+1) = \sum_{i=S}^{T} e_1 P_i(i+1) \cdot P_i(i+2) \cdots P_i(t+1), \tag{19}$$

we obtain the following key relation

$$F_{t+1}^{(S,T)} = ((\cdots(e_1 P_S(S+1) + e_1)P_S(S+2) + \cdots) + e_1)P_S(T+1) \cdots P_S(t+1). \tag{20}$$

The computation of $F_{t+1}^{(S,T)}$ becomes very easy with (20). We start from the inner most bracket. After one multiplication and one summation, we obtain a row vector whose first two elements are nonzero. The second round of multiplication and summation lead to a row vector with the first three elements being nonzero, and so on so forth. The final result is a row vector with the first $(t - S + 1)$ elements being nonzero. An efficient algorithm can be developed to implement this procedure. Obviously, the complexity of the algorithm is $O(t^2)$.

We plot the $\log - \log$ curves for $P(k, t)$ for some different m and t as shown in Figure 1, and use the least square method to fit the exponent γ and the coefficient c of the power-law under the BA model. Table 1 lists the numerical results for different m and t values. We observe that the degree exponent is independent of m and the value matches those of simulation and the analytical solution with the mean field method. The coefficient of degree distribution c is between $2m^2$ and $2m(m+1)$, again matching the theoretical value from the mean field method. Furthermore, results for $m = 3$ show that the coefficient c is independent of t, i.e., the network is stationary.
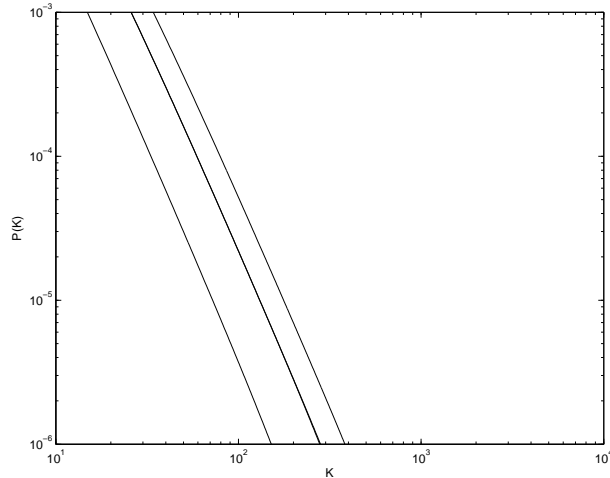

Figure 1: The degree distribution of the BA model

In Figure 1, the three lines from left to right correspond to three cases: (1) $m = 1$, $t = 150,000$; (2) $m = 3$, $t = 100,000$, $150,000$, $200,000$; (3) $m = 5$, $t = 150,000$.

The line in case (2) is the overlap of three lines corresponding to three different t values. This shows that the distribution is stationary. The three lines of the three cases are parallel, which further shows the degree exponent of the BA model is independent of m.

Table 1: Degree exponent and coefficients of the BA model

parameter m	time t	exponent γ	coefficient c
1	150000	2.960830	3.147515
3	100000	2.989636	21.79266
3	150000	2.990032	21.89667
3	200000	2.980275	21.01711
5	150000	2.978894	52.58430

3   The degree distributions of m-varying BA models

Our numerical approach is feasible and can be efficiently applied to more complex models. Since the number of edges grows faster than the number of nodes in many networks as shown by empirical evidences, we compute the degree distributions of two cases of the BA model with m-varying functions in this section.

3.1   Power function

Let the number of new links added in time step t be mt^θ, $0 \leq \theta < 1$, i.e., the new node t will link itself to mt^θ different nodes already present in the system.

We note that after t time steps, this case leads to a random network with $N = t + m_0$ nodes and approximately $\int_0^t mx^\theta dx$ links. Then, the total degree number of the system at time t is

$$\sum_j k_j \approx 2 \int_0^t mx^\theta dx = \frac{2m}{\theta + 1} t^{\theta + 1}. \tag{21}$$

Assuming continuity of $k_i(t)$, it then satisfies the following dynamic equation

$$\frac{\partial k_i}{\partial t} = mt^\theta \Pi(k_i) = mt^\theta \frac{k_i}{\sum_j k_j} = \frac{(\theta + 1)k_i}{2t}. \tag{22}$$

Under the initial condition is $k_i(t_i) = mt_i^\theta$, where t_i is the time when node i joins the network, we solve this equation and obtain

$$k_i(t) = mt_i^\theta (\frac{t}{t_i})^{\frac{1+\theta}{2}} = mt^\theta (\frac{t}{t_i})^\beta, \quad \beta = \frac{1-\theta}{2}. \tag{23}$$

Hence the degree distribution at time t

$$P(k,t) \sim \frac{2}{1-\theta} m^{\frac{2}{1-\theta}} t^z k^{-\gamma}, \quad \gamma = \frac{3-\theta}{1-\theta}, z = \frac{2\theta}{1-\theta}. \tag{24}$$

Here, z is called the non-stationary exponent. We note that this type of m-varying function was first discussed in [20].

We now construct the Markov chain for the degree sequence $\{K_i(t), t = i, i+1, ...\}$. The state space is $\Omega = \{m_i, m_i + 1, ...\}$, where $m_i = m[i^\theta]$. At time t, the probability that an existing node i will connect with the new node is given by

$$mt^\theta \frac{k_i}{\sum_j k_j} \approx \frac{(\theta + 1)k_i}{2t}. \tag{25}$$

Hence, the one-step transition probabilities are

$$p_{kj}(t+1) = P\{K_i(t+1) = j \mid K_i(t) = k\} = \begin{cases} 1 - \frac{(\theta+1)k}{2t}, & j = k \\ \frac{(\theta+1)k}{2t}, & j = k+1 \\ 0, & otherwise \end{cases} \quad (26)$$

for $k = m_i, ..., m_i + t - i$, and

$$p_{kj}(t+1) = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \quad (27)$$

for $k > m_i + t - i$. The transition probability matrix is

$$P_i(t+1) = \begin{bmatrix} 1 - \frac{m_i(\theta+1)}{2t} & \frac{m_i(\theta+1)}{2t} & & & & & \\ & 1 - \frac{(m_i+1)(\theta+1)}{2t} & \frac{(m_i+1)(\theta+1)}{2t} & & & & \\ & & \ddots & & \ddots & & \\ & & & & 1 - \frac{(m_i+t-i)(\theta+1)}{2t} & \frac{(m_i+t-i)(\theta+1)}{2t} & \\ & & & & & 1 & 0 \\ & & & & & & \ddots & \ddots \end{bmatrix}$$

$$(28)$$

for $t = i, i+1, \dots$.

We now provide the computation results when $\theta = 0.2$. We note that the structure of the transition matrices here is similar to that of (12). The difference is that now m_i is not a constant, in general, but a step function of i, as shown in Table 2.

<p style="text-align:center">Table 2:   Intervals of m_i keep constant</p>

time i	32	243	1024	3125	7776	16807	32768	59049	100000	161051
$[t^{0.2}]$	2	3	4	5	6	7	8	9	10	11

Therefore, relations (16), (17) and (18) hold for each interval, e.g., the interval $(243, 1023)$. Thus we obtain the following important result

$$F_{t+1}^{(32,t)} = F_{t+1}^{(32,242)} + F_{t+1}^{(243,1032)} + \cdots + F_{t+1}^{(59049,99999)} + F_{t+1}^{(100000,t)}. \quad (29)$$

Similarly, the initial probability distribution is $f_i(i) = (1, 0, 0, ...) = e_1$ for any i. Thus the same algorithm based on (20) can be used to compute the degree distribution $P(k,t)$ for this network.

From the computation results, we plot the $\log - \log$ curves for $P(k,t)$ for some different m and t as shown in Figure 2. We also list some numerical results in the Table 3. From the figure and the table, it is clear that this network self-organizes into a non-stationary scale-free network, with the degree exponent $\gamma \approx 3.5$.

3.2 Logarithmic function

Let the number of new links in time step t be $m \ln t$.

We note that after t time steps, the model leads to a random network with $N = t + m_0$ nodes and approximately $\int_0^t m \ln x dx$ links. Then, the total degree number of the system at time t is

$$\sum_j k_j \approx 2 \int_0^t m \ln x dx = 2mt(\ln t - 1). \quad (30)$$

Table 3:   Numerical results of the power function case

parameter m	time t	exponent γ	coefficient c
1	150000	3.502938	891.641
3	100000	3.499978	8213.46
3	150000	3.502746	10920.8
3	200000	3.496971	12300.2
5	150000	3.503176	37303.5

The average degree of the system is $\overline{k} = 2m(\ln t - 1)$, i.e., it follows a logarithmic law. There has been no analytical results for the degree distribution for this case as, we believe, it is extremely difficult if not impossible.

We now construct the Markov chain for the degree sequence $\{K_i(t), t = i, i+1, ...\}$. The state space is $\Omega = \{m_i, m_i + 1, ...\}$, where $m_i = m[\ln i]$. At time t, the probability that an existing node i will connect with the new node is given by

$$m \ln t \frac{k_i}{\sum_j k_j} \approx \frac{k_i \ln t}{2t(\ln t - 1)}. \tag{31}$$

Hence, the one-step transition probabilities are

$$p_{kj}(t+1) = P\{K_i(t+1) = j \mid K_i(t) = k\} = \begin{cases} 1 - \frac{k \ln t}{2t(\ln t - 1)}, & j = k \\ \frac{k \ln t}{2t(\ln t - 1)}, & j = k+1 \\ 0, & otherwise \end{cases} \tag{32}$$

for $k = m_i, ..., m_i + t - i$, and

$$p_{kj}(t+1) = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \tag{33}$$

for $k > m_i + t - i$. The transition probability matrix is

$$P_i(t+1) = \begin{bmatrix} 1 - \frac{m_i \ln t}{2t(\ln t - 1)} & \frac{m_i \ln t}{2t(\ln t - 1)} & & & & & \\ & 1 - \frac{(m_i+1) \ln t}{2t(\ln t - 1)} & \frac{(m_i+1) \ln t}{2t(\ln t - 1)} & & & & \\ & & \ddots & & \ddots & & \\ & & & 1 - \frac{(m_i+t-i) \ln t}{2t(\ln t - 1)} & \frac{(m_i+t-i) \ln t}{2t(\ln t - 1)} & & \\ & & & & 1 & 0 & \\ & & & & & \ddots & \ddots \end{bmatrix} \tag{34}$$

for $t = i, i+1, ...$.

We note that the structure of the transition matrices here is similar to that of (12). The difference is that now m_i is not a constant, in general, but a step function of i, as shown in Table 4.

Table 4:   Intervals of m_i keep constant

time i	21	55	149	404	1097	2981	8104	22027	59875	162755
$[\ln i]$	3	4	5	6	7	8	9	10	11	12

Therefore, relations (16), (17) and (18) hold for each interval, e.g., the interval $(404, 1096)$. Thus we obtain the following important result

$$F_{t+1}^{(21,t)} = F_{t+1}^{(21,54)} + F_{t+1}^{(55,148)} + \cdots + F_{t+1}^{(59875,162754)} + F_{t+1}^{(162755,t)}. \qquad (35)$$

Similarly, the initial probability distribution is $f_i(i) = (1, 0, 0, ...) = e_1$ for any i. Thus the same algorithm based on (20) can be used to compute the degree distribution $P(k, t)$ for this network.

From the computation results, we plot the $\log - \log$ curves for $P(k, t)$ for some different m and t as shown in Figure 3. We also list some numerical results in Table 5. From the figure and the table, it is clear that this network self-organizes into a non-stationary scale-free network, with the degree exponent $\gamma \approx 3.1$ and a positive, though very small, non-stationary exponent z.

Table 5:   Numerical results of the logarithmic function case

parameter m	time t	exponent γ	coefficient c
1	150000	3.169873	542.9149
3	100000	3.117526	1539.876
3	150000	3.081926	1722.288
3	200000	3.050253	1952.588
5	150000	3.029171	2823.681

4   Conclusions and discussions

In summary, we introduce a Markov chain-based new method to calculate degree distributions of scale-free networks numerically. Comparing with the existing analytical methods, this method is more flexible. It offers the asymptotic property of the degree distribution for the more complicated models. Using only the transition probability matrix $P_i(t+1)$, we can compute the degree distribution $P(k)$. Since the complexity of our algorithm is $O(t^2)$, its advantage over the simulation method is also quite obvious: it is fast and, for problems that it can handle, it is more reliable and provides better understanding of the network behavior.

The use of Markov chain to model the degree evolution is quite novel and opens the door for the applications of methodologies and results from a very mature field to the exciting new field of scale-free networks. For instance, we may consider to compute the joint degree distribution of a node pair by using Markov chains. Furthermore, the fact that the evolution of a complex network can be modeled by Markov chains may indicate an important direction for us to investigate the underlying mechanisms of growth networks, since we have accumulated extensive understanding of the structural properties of Markov chains as we use them to study many natural phenomena.
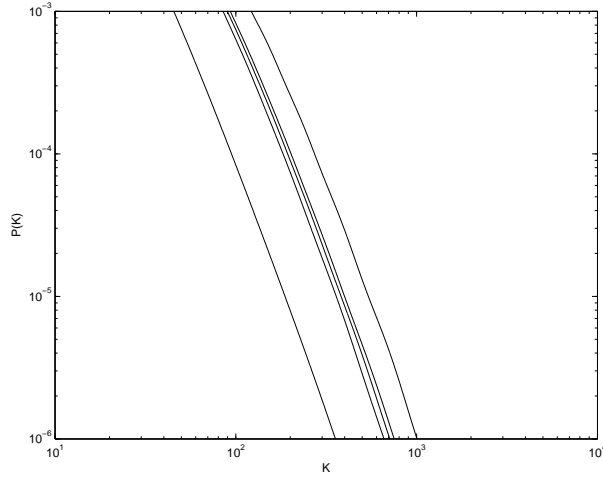
Figure 2: The degree distribution of the power function case

In Figure 2, the five lines from left to right correspond to three cases: (1) $m = 1$, $t = 150,000$; (2) $m = 3$, $t = 100,000,\ 150,000,\ 200,000$; (3) $m = 5$, $t = 150,000$. In (2), the three lines are separated, demonstrating the non-stationarity of the degree distribution. Again, we can see that the degree exponents are essentially independent of m as the lines are parallel to each other.
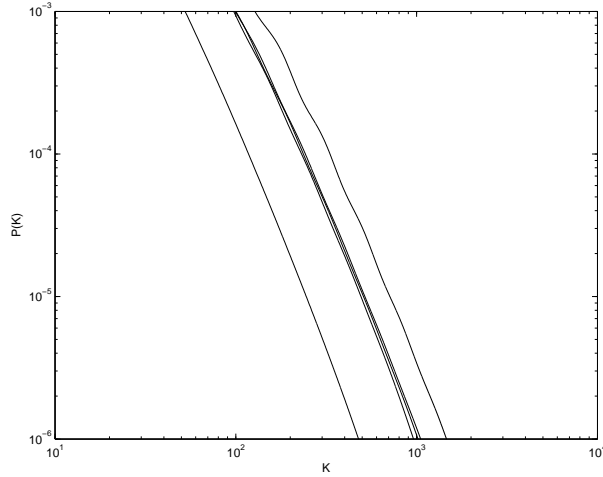

Figure 3: The degree distribution of the logarithmic function case

In Figure 3, the five lines from left to right correspond to three cases: (1) $m = 1$, $t = 150,000$; (2) $m = 3$, $t = 100,000,\ 150,000,\ 200,000$; (3) $m = 5$, $t = 150,000$. In (2), the three lines are very close to each other but not entirely overlapping, showing that while the degree distribution is not stationary, the non-stationary exponent is very small. Again, we can see that the degree exponents are essentially independent of m as the lines are parallel to each other.

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